

Polaron in t-J model

A.S. Mishchenko^{1,2} and N. Nagaosa^{1,3}

¹CREST, Japan Science and Technology Agency (JST), AIST, 1-1-1, Higashi, Tsukuba 305-8562, Japan

²RRC “Kurchatov Institute”, 123182, Moscow, Russia

³CREST, Department of Applied Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

We present numeric results for ground state and angle resolved photoemission spectra (ARPES) for single hole in t-J model coupled to optical phonons. The systematic-error free diagrammatic Monte Carlo is employed where the Feynman graphs for the Matsubara Green function in imaginary time are summed up completely with respect to phonons variables, while magnetic variables are subjected to non-crossing approximation. We obtain that at electron-phonon coupling constants relevant for high T_c cuprates the polaron undergoes self-trapping crossover to strong coupling limit and theoretical ARPES demonstrate features observed in experiment: a broad peak in the bottom of the spectra has momentum dependence which coincides with that of hole in pure t-J model.

PACS numbers: 71.10.Fd, 71.38.-k, 79.60.-i, 02.70.Ss

In the context of broad interest to the challenging properties of the high- T_c superconductors, a single hole in the Mott insulator has been studied extensively in terms of the t-J model

$$\hat{H}_{t-J} = -t \sum_{\langle ij \rangle s} c_{is}^\dagger c_{js} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \mathbf{S}_j - n_i n_j / 4), \quad (1)$$

where $c_{j\sigma}$ is projected (to avoid double occupancy) fermion annihilation operator, $n_i < 2$ is the occupation number, \mathbf{S}_i is spin-1/2 operator, and $\langle ij \rangle$ denotes nearest-neighbour sites in two-dimensional lattice. Different theoretical approaches (for review and recent studies see Refs. 1, 2, 3, 4) give consistent results for the Lehman Spectral Function (LSF) $L_{\mathbf{k}}(\omega) = -\pi^{-1} \Im G_{\mathbf{k}}(\omega)$ of the Green function $G_{\mathbf{k}}(\omega)$. Namely, the LSFs at all momenta have a quasiparticle (QP) peak in the low energy part together with a broad incoherent continuum extending up to the energy scale of the order of t . Sharp QP peak in the LSF of the ground state at momentum $\mathbf{k} = (\pi/2, \pi/2)$ has the weight $Z \sim J/t$. This QP peak is sharp at all momenta and its energy dispersion has the bandwidth $W_{J/t} \sim J$. More advanced t-t'-t''-J model takes into account long range hopping amplitudes t' and t'' which alter the bandwidth and dispersion of the QP resonance [5, 6, 7, 8, 9, 10, 11]. It was shown [5] that, depending on the parameters of the t-t'-t''-J model, the QP peak can be either enhanced or completely suppressed at a large part of the Brillouin zone. However, at parameters which are needed for description of ARPES measurements on carefully studied [12] $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ ($J/t \approx 0.4$, $t'/t \approx -0.3$, see [6, 7, 8]), the QP peak remains well defined for all momenta [5, 13, 14]. Possible damping of the peak [5], in contrast to experiment, is much less than the QP bandwidth. Therefore, the properties of QP peak in t-t'-t''-J model at realistic parameters are the same as in generic t-J model.

Experimentally, ARPES in the undoped cuprates revealed the LSF of a single hole [10, 11] and observed dispersion of the lowest peak in the LSF is in good agreement with the theoretical predictions of the t-t'-t''-J model [6, 7, 8, 9, 10, 11]. The puzzling point is that,

in contrast to the theory, experiments never show sharp QP resonance and a broad peak with the width of the order of 0.1-0.5eV ($\approx t$) is observed instead. Note, that broadening is seen just in undoped systems where the ground state of the single hole is the lowest energy state in the Hilbert space of the (N-1)-electron problem. One can rule out a possibility of an extrinsic origin of this width since the doping introduces further disorder, while a sharper peak is observed in overdoped region.

The role of electron-phonon (e-ph) coupling has gained the recent renewed interest. One reason is that the ARPES data in doped metallic cuprates revealed the energy dispersion strongly renormalized by e-ph interaction [11]. Besides, the strong e-ph interaction is crucial for explanation of renormalization and lineshapes of phonons observed in neutron scattering experiments [15, 16]. In addition, the large isotope effect on T_c for underdoped cuprates and on the superfluid density at the optimal doping suggests the vital role of e-ph coupling [17].

Strong and intermediate coupling regimes of e-ph interaction in t-J model can not be studied neither by exact diagonalization [18] on small clusters nor by self consistent Born approximation (SCBA) where both magnon and phonon propagators are subjected to non crossing approximation (NCA) which neglects the vertex corrections [13, 19, 20]. Small system size implies a discrete spectrum and, hence, neither crossover from large to small size polaron nor the problem of linewidth in ARPES can be addressed in the former approach. The latter method omits the Feynman diagrams with mutual crossing of phonon propagators and, hence, neglects the vortex corrections which are crucial for treating the e-ph interaction in the strong coupling regime (SCR). One can use the NCA for the interaction of the hole with magnetic system because spin $S=1/2$ can not flip more than one time and magnon cloud around the hole saturates. To the contrary, phonon-phonon non-crossing approximation (PPNCA) fails for SCR since number of phonon quanta around the hole is not limited.

The key role of the vortex corrections for e-ph interaction in SCR can be demonstrated by numerically ex-

act Diagrammatic Monte Carlo (DMC) method [21, 22, 23, 24] where Feynman graphs for the Matsubara Green function of a hole in phonon bath are generated by Monte Carlo and summed up without systematic errors. In the framework of this technique one can compare results of complete summation of Feynman expansion with those of restricted summation where diagrams with inter-crossing of phonon propagators are neglected. In order to extract the effect of vortex corrections on results we considered conventional two dimensional Holstein model, where the complete and PPNCA summation of Feynman expansion by DMC can be performed exactly. In this model hole freely hops with the amplitude t (t is set to unity below) and interacts with dispersionless (frequency $\Omega = \text{const}$) optical phonons by short range coupling γ

$$\hat{H}^{\text{e-ph}} = \Omega \sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + N^{-1} \gamma \sum_{\mathbf{k}, \mathbf{q}} \left[h_{\mathbf{k}}^{\dagger} h_{\mathbf{k}-\mathbf{q}} b_{\mathbf{k}} + h.c. \right]. \quad (2)$$

Exact and PPNCA results for energy and Z -factor of polaron are in good agreement at small values $g \leq 0.2$ of dimensionless interaction constant $g = \gamma^2/(8t\Omega)$ while are crucially different in the intermediate and strong coupling regimes. E.g., for $\Omega/t = 0.1$ exact result shows crossover to SCR at $g > g_H^c \approx 0.6$ while in PPNCA the polaron is in weak coupling regime even for $g = 60$. We conclude that DMC is the only method which can treat intermediate and strong coupling regime of the e-ph interaction for the problem of one hole in the macroscopic system.

In this Letter we present a study of a single hole in t-J model interacting with dispersionless optical phonons (2) by DMC [21, 22, 23, 24] method. We found that due to slowing down of the hole by spin flip cloud around it, the hole in t-J model is subject to the stronger e-ph coupling than the freely propagating hole and hence undergoes the crossover to SCR at smaller coupling. This is in contrast to the naive expectation that the small Z factor reduces the e-ph coupling in t-J model. Besides, we found that SCR occurs at e-ph couplings which are typical for high T_c materials. Finally, our results for SCR qualitatively reproduce data of ARPES experiments: a *broad peak, whose energy dispersion is similar to that of pure t-J model*, dominates in low energy part of LSF.

In the standard spin-wave approximation in momentum representation [25] the dispersionless hole $\varepsilon_0 = \text{const}$ (annihilation operator is $h_{\mathbf{k}}$) propagates in the magnon (annihilation operator is $\alpha_{\mathbf{k}}$) bath

$$\hat{H}_{\text{t-J}}^0 = \sum_{\mathbf{k}} \varepsilon_0 h_{\mathbf{k}}^{\dagger} h_{\mathbf{k}} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \quad (3)$$

with magnon dispersion $\omega_{\mathbf{k}} = 2J\sqrt{1-\gamma_{\mathbf{k}}^2}$, where $\gamma_{\mathbf{k}} = (\cos k_x + \cos k_y)/2$. The hole is scattered by magnons

$$\hat{H}_{\text{t-J}}^{\text{h-m}} = N^{-1} \sum_{\mathbf{k}, \mathbf{q}} M_{\mathbf{k}, \mathbf{q}} \left[h_{\mathbf{k}}^{\dagger} h_{\mathbf{k}-\mathbf{q}} \alpha_{\mathbf{k}} + h.c. \right] \quad (4)$$

with the scattering vortex $M_{\mathbf{k}, \mathbf{q}} = 4t(u_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}} + v_{\mathbf{q}}\gamma_{\mathbf{k}})$, where $u_{\mathbf{k}} = \sqrt{(1+\nu_{\mathbf{k}})/(2\nu_{\mathbf{k}})}$, $v_{\mathbf{k}} =$

$-sign(\gamma_{\mathbf{k}})\sqrt{(1-\nu_{\mathbf{k}})/(2\nu_{\mathbf{k}})}$, and $\nu_{\mathbf{k}} = \sqrt{1-\gamma_{\mathbf{k}}^2}$. We chose the value $J/t = 0.3$ at which NCA for magnons is shown to be sufficiently good approximation [25] and set the phonon frequency $\Omega = 0.1$ to make it similar to experimental value.

We generate Feynman expansion of Matsubara Green function of a hole in momentum representation for the infinite system at zero temperature by DMC [22, 23, 24]. Then we obtain LSF by stochastic optimization method [22, 26] which resolves equally well both sharp and broad features of the spectra. Diagrams with crossing of a magnon propagator by both magnon and phonon lines are neglected [27] though the diagrams with inter-crossing of phonon propagators are taken into account. The DMC algorithm for pure t-J model eqs. (3-4) is equivalent to the macroscopic limit of SCBA approach on finite lattices [25]. When PPNCA is introduced to DMC at finite couplings to phonons, the algorithm is nothing but the thermodynamic limit of SCBA approach on finite lattices to the complete model (2-4) when both magnons and phonons are taken into account in NCA [20]. Comparison of our data with results of Refs. [20, 25] shows that Z -factor and energy of the lowest peak are weakly influenced by finite size corrections since the relative discrepancy is less than 10^{-2} . The shapes of LSF in SCBA approach are very similar to those obtained by DMC. We observed only slight discrepancy in widths and energies of high energy peaks. Therefore, the main advantage of DMC over other existing methods is the possibility to take into account phonon-phonon vertex corrections in macroscopic system.

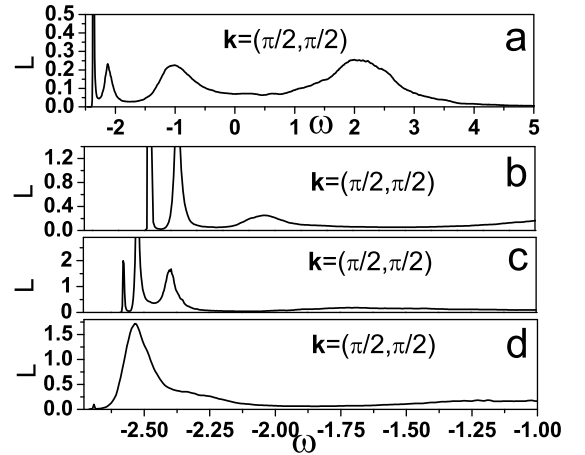


FIG. 1: Hole LSF in ground state at $J/t = 0.3$: (a) for $g = 0$; (b-d) low energy part for $g=0.1445$ [$\gamma = 0.34$] (b), $g=0.2$ [$\gamma = 0.2$] (c), and $g=0.231125$ [$\gamma = 0.43$] (d).

Figure 1 presents our results for LSF in the ground state. Three low energy peaks for $g = 0$ (Fig. 1a) are string resonances [28] since their energies, as we found in calculations of LSF for different exchange constants $0.1 \leq J \leq 0.4$, obey the scaling law $a + b_i(J/t)^{2/3}$ ($a = -3.13$, $b_{1,2,3} = 4.89/2.09/1.63$). With increasing of g these peaks are observed up to $g = 0.21$ (Figs. 1b and 1c) while the peak with highest energy broadens and

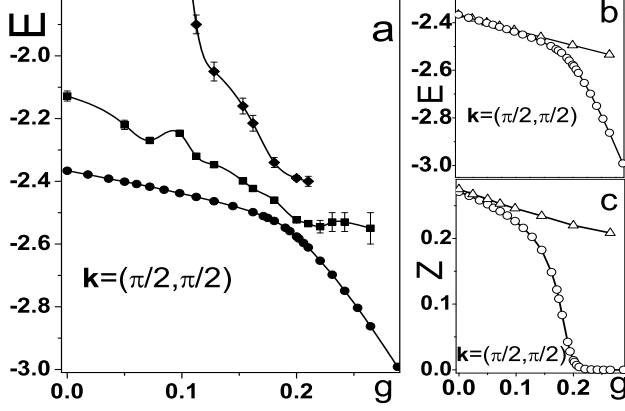


FIG. 2: Dependence on coupling strength at $J/t = 0.3$: (a) energies of lowest LSF resonances; (b [c]) energy [Z-factor] of lowest peak in DMC (circles) and PPNCA (triangles). Lines are to guide an eye. The errorbar, if not shown, is less than the point size.

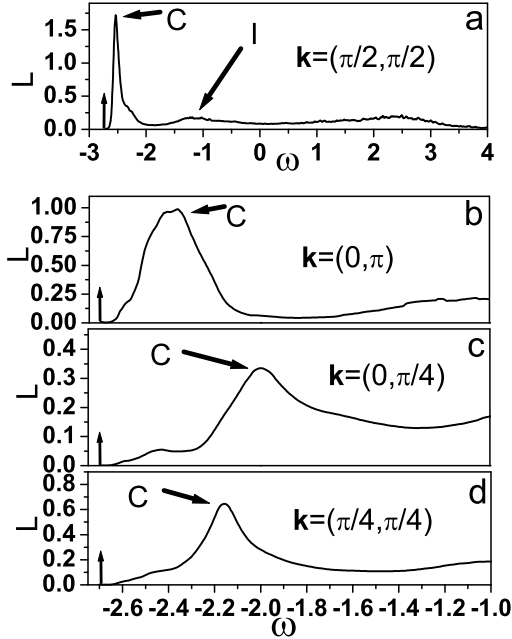


FIG. 3: LSF of the hole at $J/t = 0.3$ and $g = 0.231125$: (a) full energy range for $\mathbf{k} = (\pi/2, \pi/2)$; (b-d) low energy part for different momenta. Slanted arrows show broad peaks which can be interpreted in ARPES spectra as coherent (C) and incoherent (I) part. Vertical arrows indicate position of ground state resonance which is not seen in the vertical scale of the figure.

disappears at higher couplings (Fig. 1d).

Dependence of the peak energies (Fig. 2a) and ground state Z-factor (Fig. 2c) on g resembles picture inherent in self-trapping phenomenon [26, 29]: the states cross and hybridize at critical coupling $g_{t-J}^c \approx 0.19$ and Z-factor of ground state resonance rapidly decreases. We note, that PPNCA result does not show transition into SCR even at considerably larger g (see Fig. 2b and Fig. 2c). According to general understanding of self-trapping crossover,

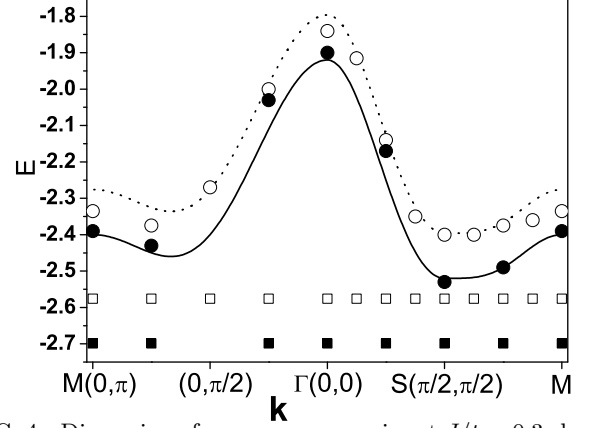


FIG. 4: Dispersion of resonances energies at $J/t = 0.3$: broad resonance (filled circles) and lowest polaron resonance (filled squares) at $g = 0.231125$; third broad resonance (open circles) and lowest polaron resonance (open squares) at $g = 0.2$. The solid curves are dispersions (5) of a hole in pure t-J model at $J/t = 0.3$ ($W_{J/t=0.3} = 0.6$): $\epsilon_{min} = -2.396$ ($\epsilon_{min} = -2.52$) for solid (dotted) line.

at small g the ground state is weakly coupled to phonons while excited resonances have strong lattice deformation. At critical coupling the crossing and hybridization of these states occurs and for higher g the roles of these states exchange: the lowest state is strongly trapped by lattice deformation while the upper ones are nearly free. Therefore, above the crossover point $g > g_{t-J}^c$ one expects that the lowest state should be dispersionless while the upper resonances have to show considerable momentum dependence. This assumption is supported by momentum dependence of LSF well above the crossover point (Fig. 3). The energy of the lowest peak is momentum independent while the bandwidth of the upper broad resonance (Fig. 4) is the same ($W_{J/t=0.3} = 0.6$) as it is in the pure t-J model. The most surprising peculiarity of the momentum dependence of broad resonance is that it is exactly the same as expected for t-J model with no coupling to phonons: it obeys the scaling relation

$$\epsilon_{\mathbf{k}} = \epsilon_{min} + W_{J/t} \{ [\cos k_x + \cos k_y]^2 / 5 + [\cos(k_x + k_y) + \cos(k_x - k_y)]^2 / 4 \}, \quad (5)$$

which describes dispersion for pure t-J model in the broad range of exchange constants $0.1 \leq J/t \leq 0.9$ [30]. We emphasize, that unrenormalized dispersion of the upper resonances is the general property of SCR. E.g., for the coupling $g = 0.2$, which is slightly higher than the critical coupling g_{t-J}^c , (see Fig. 1c and 2), dispersion of the upper resonance also obeys eqs. (5) while the lowest peak is momentum independent (see Fig. 4).

The behavior of LSF in SCR is exactly the same as it is observed in ARPES experiments. The LSF consists of *broad QP* peak and high-energy incoherent continuum (see Fig. 3). Besides, momentum dependence of the broad QP peak is similar to dispersion of sharp resonance in the pure t-J model (see Fig. 4). The lowest

lying dispersionless peak in SCR has small Z -factor and can not be discerned in ARPES experiments: its spectral weight is small ($Z \sim 0.015$) at $g = 0.2$ (Fig. 1c) and completely suppressed ($Z < 10^{-3}$) at $g = 0.231125$ (Fig. 1d). On the other hand, the momentum dependence of spectral weight Z' of broad dispersive resonance in SCR is akin to that in pure t-J model. For $g = 0.231125$ the weights of broad peak at $\mathbf{k} = (\pi/2, \pi/2)$ (~ 0.27) and at $\mathbf{k} = (0, 0)$ (~ 0.05) coincide with Z -factors of sharp resonances at corresponding momenta in pure t-J model. Our calculation show that this similarity is the robust feature of SCR: $Z'_{(\pi/2, \pi/2)} \sim 0.27 \pm 0.01$ and $Z'_{(0,0)} \sim 0.05 \pm 0.005$ in the broad range of coupling constants $0.21 < g < 0.27$.

Comparing the critical interaction $g_{t-J}^c \approx 0.19$ for the hole in t-J model and critical coupling $g_H^c \approx 0.6$ for Holstein model with the same value of hopping t , we conclude that interaction with spins enhances e-ph coupling and accelerates transition into SCR. Emission of magnons on each hopping shrinks the bandwidth of lowest lying resonance by the factor of J/t while the reduction of e-ph vertex by the factor Z seems to be absent. This makes the influence of e-ph interaction on low energy part of LSF more effective. We emphasize that the critical interaction for transition to SCR is low enough for t-J model

to bring the realistic system into SCR. E.g., theoretical estimate of the interaction strength from the fitting of phonon energies and lineshapes to neutron scattering experiment gives rather large magnitude for e-ph coupling in La(Sr)CuO₄ [15, 16]. Since the interaction vertex is momentum dependent in the model [15, 16], we can establish only lower and upper bound for effective coupling g in our model with short-range interaction. The averaging over the Brillouin zone gives the lower bound $g_{\text{exp}}^{\text{min}} \geq 0.15$ while the maximal value at the Brillouin zone boundary determines the upper bound $g_{\text{exp}}^{\text{max}} \leq 0.5$. However, since self-trapping is governed mainly by short-range coupling [29], effective constant in our model is more close to the upper bound $g_{\text{exp}}^{\text{max}}$. Thus, realistic high T_c cuprates are expected to be in SCR.

Finally, we conclude that puzzling behavior of ARPES spectra in undoped high T_c materials, which manifests oneself in unexpectedly *broad* quasiparticle peak with dispersion corresponding to pure Mott insulator model, is driven by strong electron-phonon interaction.

Fruitful discussions with N. V. Prokof'ev, B. V. Svistunov, G. Khaliullin and G. A. Sawatzky are acknowledged. This work was supported by RFBR 01-02-16508.

-
- [1] C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).
 - [2] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991); E. Dagotto, *ibid.* **66**, 763 (1994).
 - [3] M. Brunner, F. F. Assaad, and A. Muramatsu, Phys. Rev. B **62**, 15480 (2000).
 - [4] A. S. Mishchenko, N. V. Prokof'ev, and B. V. Svistunov, Phys. Rev. B **64**, 033101 (2001).
 - [5] J. Bala, A. M. Oleś, and J. Zaanen, Phys. Rev. B **52**, 4597 (1995).
 - [6] T. Xiang and M. Wheatley, Phys. Rev. B **54**, R12653 (1996).
 - [7] B. Kyung and R. A. Ferrell, Phys. Rev. B **54**, 10125 (1996).
 - [8] T. K. Lee and C. T. Shih, Phys. Rev. B **55**, 5983 (1997).
 - [9] T. K. Lee, C-M. Ho, and N. Nagaosa, Phys. Rev. Lett. **90**, 067001 (2003).
 - [10] T. Tohyama and S. Maekawa, Superconductors Science and Technology **13**, R17 (2000).
 - [11] A. Danmascelli, Z.-X. Shen, and Z. Hussain, Rev. Mod. Phys. **75**, 473 (2003).
 - [12] B. O. Wells, Z.-X. Shen, A. Matsuura, D. M. King, M. A. Kastner, M. Greven, and R. G. Birgenau, Phys. Rev. Lett. **74**, 964 (1995).
 - [13] S. Yunoki, A. Macridin, and G. A. Sawatzky, private communication, unpublished
 - [14] A. S. Mishchenko and N. Nagaosa, unpublished.
 - [15] P. Horsch and G. Khaliullin, in *Open Problems in Strongly Correlated Electron Systems*, J. Bonca et. al. (eds.), Kluwer-Academic, Boston, p. 81 (2001).
 - [16] P. Horsch, G. Khaliullin, and V. Oudovenko, Physica C **341-348**, 117 (2000).
 - [17] J. Hofer, K. Conder, T. Sasagawa, Guo-meng Zhao, M. Willemin, H. Keller, and K. Kishio, Phys. Rev. Lett. **84**, 4192 (2000).
 - [18] B. Bauml, G. Wellein, and H. Fehske, Phys. Rev. B **58**, 3663 (1998).
 - [19] A. Ramsak, P. Horsch, and P. Fulde, Phys. Rev. B **46**, 14305 (1992).
 - [20] B. Kyung, S. I. Mukhin, V. N. Kostur, and R. A. Ferrel, Phys. Rev. B **54**, 13167 (1996).
 - [21] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **81**, 2514 (1998).
 - [22] A.S. Mishchenko, N.V. Prokof'ev, A. Sakamoto, and B.V. Svistunov, Phys. Rev. B **62**, 6317 (2000).
 - [23] A. S. Mishchenko and N. Nagaosa, Phys. Rev. Lett. **86**, 4624 (2001).
 - [24] A. S. Mishchenko, N. Nagaosa, N. V. Prokof'ev, B. V. Svistunov, and E. A. Burovskii, J. Nonlinear Opt. **29**, 257 (2002).
 - [25] Z. Liu and E. Manousakis, Phys. Rev. B **45**, 2425 (1992).
 - [26] A.S. Mishchenko, N. Nagaosa, N.V. Prokof'ev, A. Sakamoto, and B.V. Svistunov, Phys. Rev. B **66**, 020301 (2002).
 - [27] To avoid sign problem arising from the momentum dependence of magnon scattering vertex $M_{\mathbf{k},\mathbf{q}}$.
 - [28] B. I. Shraiman and E. Sigg, Phys. Rev. Lett. **60**, 740 (1988).
 - [29] E. I. Rashba, *Self-Trapping of Excitons*, in *Modern Problems in Condensed Matter Sciences*, Edited by V. M. Agranovich and A. A. Maradudin (North-Holland, Amsterdam, 1982), Vol. 2, p. 543.
 - [30] F. Marsiglio, A. E. Ruckenstein, S. Schmitt-Rink and C. M. Varma, Phys. Rev. B **43**, 10882 (1991).